

USE OF GENERALIZED INVERSES IN LINEAR MODEL THEORY

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Abstract

Expectations and variances of some quadratic forms arising in the application of Henderson's Method III of estimating variance components are obtained. Possible extensions are indicated.

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0. Introduction

Discussion of the general linear model

$$(1) \quad \underline{Y} = X\underline{\beta} + \underline{\epsilon}, \mathcal{E}(\underline{\epsilon}) = \underline{0}, \text{Var } \underline{\epsilon} = I_{\sigma}^2$$

where \underline{Y} is an $n \times 1$ vector of observable random variables, X is an $n \times p$ matrix of known constants, $\underline{\beta}$ is a $p \times 1$ vector of unknown parameters and $\underline{\epsilon}$ is an $n \times 1$ vector of unobservable random variables has been facilitated by use of generalized inverses. In this paper we consider the expectations, variances and covariances of "sums of squares" arising in the "analysis of variance" under a model of the form (1). Assumptions about $\underline{\beta}$ are varied so as to include the classical "fixed", "mixed" and "random" models. Section 1 reviews the use of generalized inverses in the treatment of the general linear model. Section 2 deals with (1) in the partitioned form $\underline{Y} = X_1\underline{\beta}_1 + X_2\underline{\beta}_2 + \underline{\epsilon}$ and sums of squares arising in the analysis of variance of such a model are investigated under the fixed, mixed and random model assumptions. Section 3 provides a trivial, though important extension of the results of Section 2 to the model $\underline{Y} = X_1\underline{\beta}_1 + X_2\underline{\beta}_2 + X_3\underline{\beta}_3 + \underline{\epsilon}$ which include as special cases the work of Searle (5).

1. Use of Generalized Inverses in Linear Model Theory

Recent papers by Rao (4), unpublished notes of Bose (1) and the book by Rao (3) have indicated that generalized inverses can greatly simplify and unify treatment of the "less than full rank" linear model or the analysis of variance model. Recall that A^g is said to be a generalized inverse of A if $AA^gA = A$ and that the consistent equations $A\underline{b} = \underline{g}$ have the general solution

$$\underline{b} = A^g \underline{g} + (I - A^g A) \underline{z}$$

where \underline{z} is an arbitrary vector. Since the normal or least squares equations

$$(2) \quad X'X\underline{b} = X'y$$

for estimating \underline{b} in the model (1) are always consistent it follows that the general solution to the normal equations (2) is

$$(3) \quad \underline{b} = (X'X)^G X'y + [I - (X'X)^G X'X]\underline{z}$$

where \underline{z} is an arbitrary vector. Invariance of $X\underline{b}$, the projection of y on the column space of X is provided by the following Lemma due to Bose.

Lemma 1: Let $D = I - X(X'X)^G X'$. Then

$$(a) \quad DX = \underline{0}$$

(b) D is unique, symmetric and idempotent

Proof: Since $(X'X)^G$ is a generalized inverse of $X'X$ we have $X'DD'X = \underline{0}$ or $X'D = \underline{0}$.

If $D_1 = I - X(X'X)_1^G X'$ and $D_2 = I - X(X'X)_2^G X'$ then $(D_1 - D_2)'(D_1 - D_2) = [(X'X)_1^G X' - (X'X)_2^G X']^2 X'(D_1 - D_2) = \underline{0}$ so that $D_1 = D_2$ and hence D is unique. Since $D' = I - X(X'X)^G X'$ and $(X'X)^G$ is a generalized inverse of $X'X$ it follows that D is symmetric and hence also that $DX = \underline{0}$. Since $D^2 = [I - X(X'X)^G X']D$ idempotency follows from $X'D = \underline{0}$.

Note that $X(X'X)^G X'$ is also unique, symmetric and idempotent, idempotency following from $X(X'X)^G X'D = \underline{0}$.

It is clear from Lemma 1 that $X\underline{b}$ is uniquely determined whatever generalized inverse or solution to the normal equations is used. A linearly estimable function (Bose [1]) of $\underline{\beta}$ is one for which \underline{c}' exists so that $\underline{c}'X = \underline{\ell}'$. It follows that estimates of linearly estimable functions are unique since

$$\underline{\ell}'\underline{\hat{\beta}} = \underline{\ell}'\underline{b} = \underline{c}'X(X'X)^G X'y$$

is unique.

Lemma 2: Rank $X(X'X)^G X' = \text{Tr}[X(X'X)^G X'] = \text{Rank}(X'X)$

Proof: Since $X(X'X)^G X'$ is idempotent and symmetric its rank equals its trace.

Also $\text{Rank } X(X'X)^G X' = \text{Rank } (X'X) (X'X)^G$ so that $\text{Rank } (X'X) \leq \text{Rank } (X'X) (X'X)^G \leq \text{Rank } (X'X) (X'X)^G (X'X) = \text{Rank } (X'X)$ or $\text{Rank } (X'X) = \text{Rank } X(X'X)^G X'$.

The analysis of variance associated with the model (1) thus takes the form

<u>Source</u>	<u>D.F.</u>	<u>Sum of Squares</u>
Regression on $\underline{\beta}$	$\text{Rank } X'X$	$SS(\underline{\beta}) = \underline{y}' X (X'X)^G X' \underline{y}$
Error	$n - \text{Rank } (X'X)$	$SSE = \underline{y}' [I - X(X'X)^G X'] \underline{y}$

From Lemma 1 the sums of squares are unique. The degrees of freedom are the ranks of the matrices of the quadratic forms.

If \underline{Y} has a multivariate normal distribution with $E\underline{Y} = \underline{\mu}$ and $\text{Var } \underline{Y} = V$ then it is well known (Rao [2]) that

$$\begin{aligned}
 E[\underline{Y}' B \underline{Y}] &= \underline{\mu}' B \underline{\mu} + \text{Tr}(BV) \\
 \text{Var}[\underline{Y}' B \underline{Y}] &= 4 \underline{\mu}' B V B \underline{\mu} + 2 \text{Tr}(BV)^2 \\
 \text{Cov}[\underline{Y}' B \underline{Y}, \underline{Y}' C \underline{Y}] &= 4 \underline{\mu}' B V C \underline{\mu} + 2 \text{Tr}(BVCV)
 \end{aligned}$$

(4)

Using these results it is easy to verify that under the additional assumption that $\underline{Y} \sim N(X\underline{\beta}, I\sigma^2)$ we have

$$\begin{aligned}
 E[SS\underline{\beta}] &= \underline{\beta}' X' X \underline{\beta} + \sigma^2 \text{Rank } (X'X) ; \text{Var } (SS\underline{\beta}) = 4 \underline{\beta}' X' X \underline{\beta} + 2\sigma^4 \text{Rank } (X'X) \\
 E[SSE] &= \sigma^2 [n - \text{Rank } X'X] ; \text{Var } (SSE) = 2\sigma^4 [n - \text{Rank } (X'X)] \\
 \text{Cov } (SSE, SS\underline{\beta}) &= 0
 \end{aligned}$$

2. The model $\underline{Y} = X_1 \underline{\beta}_1 + X_2 \underline{\beta}_2 + \underline{\epsilon}$

In this section we discuss the model

$$(2.0) \quad \underline{Y} = X_1 \underline{\beta}_1 + X_2 \underline{\beta}_2 + \underline{\epsilon}, E[\underline{\epsilon}] = \underline{0}, \text{Var } [\underline{\epsilon}] = I\sigma^2$$

where

X_1 is an $n \times q$ matrix of known constants

X_2 is an $n \times (p-q)$ matrix of known constants

$\underline{\beta}_1$ is a $q \times 1$ vector of unknown parameters

$\underline{\beta}_2$ is a $(p-q) \times 1$ vector of unknown parameters

and \underline{Y} and $\underline{\epsilon}$ are as used in model (1).

The model (2.0) will be discussed under the following assumptions on the parameters $\underline{\beta}_1$ and $\underline{\beta}_2$.

Assumption A: $\underline{\beta}_1$ and $\underline{\beta}_2$ are "fixed" vectors of parameters

Assumption B: $\underline{\beta}_1$ is a fixed vector of parameters while $\underline{\beta}_2$ is a random vector of parameters with $\mathcal{E}[\underline{\beta}_2] = \underline{0}$ and

$$\text{Var} \begin{bmatrix} \underline{\beta}_2 \\ \epsilon \end{bmatrix} = \begin{bmatrix} I\sigma_2^2 & 0 \\ 0 & I\sigma^2 \end{bmatrix}$$

Assumption C: $\underline{\beta}_1$ and $\underline{\beta}_2$ are random vectors of parameters with

$$\mathcal{E} \begin{bmatrix} \underline{\beta}_1 \\ \underline{\beta}_2 \end{bmatrix} = \begin{bmatrix} \underline{0} \\ \underline{0} \end{bmatrix} \text{ and}$$

$$\text{Var} \begin{bmatrix} \underline{\beta}_1 \\ \underline{\beta}_2 \\ \underline{\epsilon} \end{bmatrix} = \begin{bmatrix} I\sigma_1^2 & 0 & 0 \\ 0 & I\sigma_2^2 & 0 \\ 0 & 0 & I\sigma^2 \end{bmatrix}$$

Using the usual terminology the model (2.0) under assumption A is called a "fixed" model, the model (2.0) under assumption B is called a "mixed" model and that under C is called a "random" model.

The first step in the analysis of model (2.0) consists of finding expressions for the sums of squares used in the analysis of variance, namely, the sum of squares for error, the sum of squares for $\underline{\beta}_2$ after adjusting for $\underline{\beta}_1$ and the sum of squares for $\underline{\beta}_1$ ignoring $\underline{\beta}_2$.

The normal equations for the model (2.0) in partitioned form are

$$(2.1) \quad \begin{bmatrix} X_1' X_1 & X_1' X_2 \\ X_2' X_1 & X_2' X_2 \end{bmatrix} \begin{bmatrix} \underline{b}_1 \\ \underline{b}_2 \end{bmatrix} = \begin{bmatrix} X_1' y \\ X_2' y \end{bmatrix}$$

where \underline{b}_1 and \underline{b}_2 denote estimates of β_1 and β_2 respectively. Multiplying both sides of (2.1) by

$$\begin{bmatrix} I & 0 \\ -X_2' X_1 (X_1' X_1)^{-1} & I \end{bmatrix}$$

yields the reduced normal equations,

$$(2.2) \quad \begin{bmatrix} X_1' X_1 & X_1' X_2 \\ 0 & X_2' D_1 X_2 \end{bmatrix} \begin{bmatrix} \underline{b}_1 \\ \underline{b}_2 \end{bmatrix} = \begin{bmatrix} X_1' y \\ X_2' D_1 y \end{bmatrix}$$

where $D_1 = I - X_1 (X_1' X_1)^{-1} X_1'$. Recall that from Lemma 1, $D_1 X_1 = 0$. It follows from (2.2) that

$$\begin{aligned} \underline{b}_1 &= (X_1' X_1)^{-1} [X_1' y - (X_1' X_2) (X_2' D_1 X_2)^{-1} X_2' D_1 y] \\ \underline{b}_2 &= (X_2' D_1 X_2)^{-1} X_2' D_1 y \end{aligned}$$

The sum of squares for regression is thus

$$\begin{aligned} SSR &= y' X \underline{b} = y' X_1 \underline{b}_1 + y' X_2 \underline{b}_2 \\ &= y' X_1 (X_1' X_1)^{-1} X_1' y - y' X_1 (X_1' X_1)^{-1} X_1' X_2 (X_2' D_1 X_2)^{-1} X_2' D_1 y \\ &\quad + y' X_2 (X_2' D_1 X_2)^{-1} X_2' D_1 y \end{aligned}$$

$$= \underline{y}' \underline{X}_1 (\underline{X}'_1 \underline{X}_1)^G \underline{X}'_1 \underline{y} + \underline{y}' \underline{D}_1 \underline{X}_2 (\underline{X}'_2 \underline{D}_1 \underline{X}_2)^G \underline{X}'_2 \underline{D}_1 \underline{y}$$

Note that $\underline{y}' \underline{X}_1 (\underline{X}'_1 \underline{X}_1)^G \underline{X}'_1 \underline{y}$ is the sum of squares for regression which would have been obtained had we fitted the model $\underline{y} = \underline{X}_1 \underline{\beta}_1 + \underline{\epsilon}$ i.e. had we ignored $\underline{\beta}_2$.

Hence we call $\underline{y}' \underline{X}_1 (\underline{X}'_1 \underline{X}_1)^G \underline{X}'_1 \underline{y}$ the sum of squares due to $\underline{\beta}_1$ ignoring $\underline{\beta}_2$ written $SS_{\underline{\beta}_1}$. We call $\underline{y}' \underline{D}_1 \underline{X}_2 (\underline{X}'_2 \underline{D}_1 \underline{X}_2)^G \underline{X}'_2 \underline{D}_1 \underline{y}$ the sum of squares due to $\underline{\beta}_2$ after "adjusting for $\underline{\beta}_1$ " written $SS(\underline{\beta}_2/\underline{\beta}_1)$. Thus

$$SSR = SS_{\underline{\beta}_1} + SS(\underline{\beta}_2/\underline{\beta}_1)$$

The error sum of squares is

$$SSE = \underline{y}' [I - X(X'X)^G X'] \underline{y} = \underline{y}' \underline{y} - \underline{y}' \underline{X}_1 \underline{b}_1 - \underline{y}' \underline{X}_2 \underline{b}_2$$

$$= \underline{y}' [I - \underline{X}_1 (\underline{X}'_1 \underline{X}_1)^G \underline{X}'_1 - \underline{D}_1 \underline{X}_2 (\underline{X}'_2 \underline{D}_1 \underline{X}_2)^G \underline{X}'_2 \underline{D}_1]$$

The analysis of variance for the model (2.0) thus takes the form

<u>Source</u>	<u>D.F.</u>	<u>Sum of Squares</u>
$\underline{\beta}_1$ (ignoring $\underline{\beta}_2$)	Rank $\underline{X}'_1 \underline{X}_1$	$SS_{\underline{\beta}_1} = \underline{y}' \underline{X}_1 (\underline{X}'_1 \underline{X}_1)^G \underline{X}'_1 \underline{y}$
$\underline{\beta}_2$ (adjusted for $\underline{\beta}_1$)	Rank $\underline{X}'_2 \underline{D}_1 \underline{X}_2$	$SS(\underline{\beta}_2/\underline{\beta}_1) = \underline{y}' \underline{D}_1 \underline{X}_2 (\underline{X}'_2 \underline{D}_1 \underline{X}_2)^G \underline{X}'_2 \underline{D}_1 \underline{y}$
Error	$n - \text{Rank } X'X$	$SSE = \underline{y}' [I - \underline{X}_1 (\underline{X}'_1 \underline{X}_1)^G \underline{X}'_1 - \underline{D}_1 \underline{X}_2 (\underline{X}'_2 \underline{D}_1 \underline{X}_2)^G \underline{X}'_2 \underline{D}_1] \underline{y}$

Table 2.1 gives the expectations of the sums of squares for the model (2.0) under assumptions A, B and C while Table 2.2 gives the variances and covariances of the sums of squares for the model (2.0) again under assumptions A, B and C. To illustrate the simple and routine form of the computations we derive the results for $SS(\underline{\beta}_2/\underline{\beta}_1)$, the results for the other expressions being derived in a similar fashion.

Under assumption A we have

$$E[SS_{\underline{\beta}_2/\underline{\beta}_1}] = [\underline{\beta}'_1/\underline{\beta}'_2] \begin{bmatrix} \underline{X}'_1 \\ \underline{X}'_2 \end{bmatrix} \underline{D}_1 \underline{X}_2 (\underline{X}'_2 \underline{D}_1 \underline{X}_2)^G \underline{X}'_2 \underline{D}_1 [\underline{X}_1 \quad \underline{X}_2] \begin{bmatrix} \underline{\beta}_1 \\ \underline{\beta}_2 \end{bmatrix}$$

$$\begin{aligned}
& + \sigma^2 \text{Tr} [D_1 X_2 (X_2' D_1 X_2) X_2' D_1] \\
& = [\beta_1' / \beta_2'] \begin{bmatrix} 0 \\ X_2' D_1 \end{bmatrix} [X_1 X_2] \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \sigma^2 \text{Rank} (X_2' D_1 X_2) \\
& = \beta_2' X_2' D_1 X_2 \beta_2 + \sigma^2 \text{Rank} X_2' D_1 X_2
\end{aligned}$$

Similarly under assumption A we have

$$\begin{aligned}
\text{Var} [SS_{\beta_2} / \beta_1] & = 4[\beta_1' / \beta_2'] \begin{bmatrix} X_1' \\ X_2' \end{bmatrix} [D_1 X_2 (X_2' D_1 X_2) X_2' D_1]^2 [X_1 / X_2] \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} \\
& \quad + 2\sigma^4 \text{Tr} [D_1 X_2 (X_2' D_1 X_2) X_2' D_1]^2 \\
& = 4\beta_2' X_2' D_1 X_2 \beta_2 \sigma^2 + 2\sigma^4 \text{Rank} X_2' D_1 X_2
\end{aligned}$$

since the matrix $D_1 X_2 (X_2' D_1 X_2) X_2' D_1$ is idempotent by Lemma 1.

Under assumption B we have

$$\begin{aligned}
E[SS(\beta_2 / \beta_1)] & = \beta_1' X_1' [D_1 X_2 (X_2' D_1 X_2) X_2' D_1] X_1 \beta_1 + \text{Tr} [D_1 X_2 (X_2' D_1 X_2) X_2' D_1 [I\sigma^2 + X_2 X_2' \sigma_2^2]] \\
& = \sigma^2 \text{Rank} (X_2' D_1 X_2) + \sigma_2^2 \text{Tr} (X_2' D_1 X_2)
\end{aligned}$$

and

$$\begin{aligned}
\text{Var} [SS_{\beta_2} / \beta_1] & = 4\beta_1' X_1' [D_1 X_2 (X_2' D_1 X_2) X_2' D_1]^2 X_1 \beta_1 \sigma^2 + 2\text{Tr} [D_1 X_2 (X_2' D_1 X_2) X_2' D_1 [I\sigma^2 + X_2 X_2' \sigma_2^2]]^2 \\
& = 2\sigma^4 \text{Rank} (X_2' D_1 X_2) + 4\sigma^2 \sigma_2^2 \text{Tr} (X_2' D_1 X_2) \\
& \quad + 2\sigma_2^4 \text{Tr} [X_2' D_1 X_2]^2
\end{aligned}$$

Under assumption C we have

$$\begin{aligned}
E[SS(\beta_2 / \beta_1)] & = \text{Tr} [D_1 X_2 (X_2' D_1 X_2) X_2' D_1 [X_1 X_1' \sigma_1^2 + X_2 X_2' \sigma_2^2 + I\sigma^2]] \\
& = \sigma^2 \text{Rank} (X_2' D_1 X_2) + \sigma_2^2 \text{Tr} (X_2' D_1 X_2)
\end{aligned}$$

and

$$\begin{aligned}
\text{Var}[SS(\beta_2 / \beta_1)] & = 2\text{Tr} \{D_1 X_2 (X_2' D_1 X_2) X_2' D_1 [X_1 X_1' \sigma_1^2 + X_2 X_2' \sigma_2^2 + I\sigma^2]\}^2 \\
& = 2\sigma^4 \text{Rank} (X_2' D_1 X_2) + 4\sigma_2^2 \sigma^2 \text{Tr} (X_2' D_1 X_2) \\
& \quad + 2\sigma_2^4 \text{Tr} (X_2' D_1 X_2)^2
\end{aligned}$$

TABLE 2.1 EXPECTATIONS OF SUMS OF SQUARES UNDER MODEL (2.0)

Coefficient of:

	Sum of Squares	D.F.	σ^2	σ_2^2	σ_1^2	β Terms
Fixed	$SS\beta_1$	Rank $X_1'X_1$	Rank $X_1'X_1$	-----	----	$\beta_1'X_1'X_1\beta_1 + 2\beta_1'X_1'X_2\beta_2 + \beta_2'X_2'X_2\beta_2 - \beta_2'X_2'D_1X_2\beta_2$
	$SS(\beta_2/\beta_1)$	Rank $X_2'D_1X_2$	Rank $X_2'D_1X_2$	-----	----	$\beta_2'X_2'D_1X_2\beta_2$
	SSE	n-Rank $X'X$	n-Rank $X'X$	----	----	-----
Mixed	$SS\beta_1$	Rank $X_1'X_1$	Rank $X_1'X_1$	$\text{Tr}(X_2'X_2) - \text{Tr}(X_2'D_1X_2)$	----	$\beta_1'X_1'X_1\beta_1$
	$SS(\beta_2/\beta_1)$	Rank $(X_2'D_1X_2)$	Rank $(X_2'D_1X_2)$	$\text{Tr}(X_2'D_1X_2)$	----	-----
	SSE	n-Rank $X'X$	n-Rank $X'X$	---	---	----
Random	$SS\beta_1$	Rank $X_1'X_1$	Rank $X_1'X_1$	$\text{Tr}(X_2'X_2) - \text{Tr}(X_2'D_1X_2)$	$\text{Tr}(X_1'X_1)$	-----
	$SS(\beta_2/\beta_1)$	Rank $(X_2'D_1X_2)$	Rank $(X_2'D_1X_2)$	$\text{Tr}(X_2'D_1X_2)$	----	----
	SSE	n-Rank $X'X$	n-Rank $(X'X)$	----	----	----

∞

$$D_1 = I - X_1(X_1'X_1)^{-1}X_1'$$

Table 2.2

VARIANCES AND COVARIANCES FOR MODEL 2.0

Sum of Squares	σ^2	σ^2	σ^2	σ^2 σ^2	σ^2 σ^2	σ^2 σ^2	β
SSE	$2[n - \text{Rank}(X'X)]$						$4\beta_2' X_2' D_1 X_2 \beta_1 \sigma^2$
$SS(\beta_2/\beta_1)$	$2 \text{Rank}(X_2' D_1 X_2)$						$4\beta_1' X_1' X_1 \beta_1 \sigma^2 + 4\beta_2 \sigma^2 X_2' X_2 \beta_2$
$SS\beta_1$	$2 \text{Rank}(X_1' X_1)$						$-4\beta_2' X_2' D_1 X_2 \beta_2 \sigma^2 + 8\beta_1' X_1' X_2 \beta_2 \sigma^2$
$SS(\beta_2/\beta_1), SSE$							
$SS(\beta_2/\beta_1), SS\beta_1$							
$SSE, SS\beta_1$							
SSE	$2[n - \text{Rank}(X'X)]$						
$SS(\beta_2/\beta_1)$	$2 \text{Rank}(X_2' D_1 X_2)$	$2\text{Tr}(X_2' D_1 X_2)^2$		$4\text{Tr}(X_2' D_1 X_2)$			
$SS\beta_1$	$2 \text{Rank}(X_1' X_1)$	$2\text{Tr}[X_2' X_1 (X_1' X_1)^{-1} X_1' X_2]^2$		$4\text{Tr}[X_2' X_1 (X_1' X_1)^{-1} X_1' X_2]$			$\sigma^2 4\beta_1' X_1' X_1 \beta_1 + \beta_1' X_1' X_2 X_2' X_1 \beta_1 \sigma^2$
$SS(\beta_2/\beta_1)$							
$SS(\beta_2/\beta_1), SS\beta_1$		$2\text{Tr}\{X_2' D_1 X_2 (X_2' X_1) (X_1' X_1)^{-1} X_1' X_2\}$					
$SS\beta_1, SSE$							

Table 2.2 (cont'd)

VARIANCES AND COVARIANCES FOR MODEL 2.0

Sum of Squares	σ^4	σ_2^4	σ_1^4	$\sigma^2\sigma_2^2$	$\sigma^2\sigma_1^2$	$\sigma_1^2\sigma_2^2$	β Terms
SSE	$2[n - \text{Rank}(X'X)]$						
$SS(\beta_2/\beta_1)$	$2 \text{Rank}(X_2'D_1X_2)$	$2\text{Tr}[X_2'D_1X_2]^2$		$4 \text{Tr}(X_2'D_1X_2)$			
$SS\beta_1$	$2 \text{Rank}(X_1'X_1)$	$2\text{Tr}[X_2'X_1(X_1'X_1)^G X_1'X_2]^2$	$2\text{Tr}[X_1'X_1]^2$	$4\text{Tr}[X_2'X_1(X_1'X_1)^G X_1'X_2]$	$4\text{Tr}[X_1'X_1]$	$4 \text{Tr}[X_1'X_2X_2'X_1]$	
$SS(\beta_2/\beta_1), \text{SSE}$							
$SS(\beta_2/\beta_1), SS\beta_1$		$2\text{Tr}[X_2'D_1X_2[X_2'X_1(X_1'X_1)^G X_1'X_2]]$					
$SS\beta_1, \text{SSE}$							

3. The model $\underline{Y} = X_1\beta_1 + X_2\beta_2 + X_3\beta_3 + \underline{\epsilon}$

In this section we consider the model

$$(3.0) \quad \underline{Y} = X_1\beta_1 + X_2\beta_2 + X_3\beta_3 + \underline{\epsilon}$$

where X_1 is an $n \times p_1$ matrix of known constants

X_2 is an $n \times p_2$ matrix of known constants

X_3 is an $n \times p_1 - p_2$ matrix of known constants

and \underline{Y} and $\underline{\epsilon}$ are as before. We make the assumption that $E[\underline{Y}] = X_1\beta_1$, and that

$$\begin{bmatrix} \beta_2 \\ \beta_3 \\ \underline{\epsilon} \end{bmatrix} \text{ has a } N \left(\underline{0}, \begin{bmatrix} I\sigma_2^2 & \underline{0} & \underline{0} \\ \underline{0} & I\sigma_1^2 & \underline{0} \\ \underline{0} & \underline{0} & I\sigma^2 \end{bmatrix} \right) \text{ distribution. The theory developed in}$$

Section 2 allows the results of that section to be extended easily.

The normal equations for the model (3.0) in partitioned form are

$$(3.1) \quad \begin{bmatrix} X_1'X_1 & X_1'X_2 & X_1'X_3 \\ X_2'X_1 & X_2'X_2 & X_2'X_3 \\ X_3'X_1 & X_3'X_2 & X_3'X_3 \end{bmatrix} \begin{bmatrix} \underline{b}_1 \\ \underline{b}_2 \\ \underline{b}_3 \end{bmatrix} = \begin{bmatrix} X_1'\underline{y} \\ X_2'\underline{y} \\ X_3'\underline{y} \end{bmatrix}$$

Multiplying both sides (3.1) by

$$\begin{bmatrix} I & \underline{0} & \underline{0} \\ -X_2'X_1(X_1'X_1)^G & I & \underline{0} \\ -X_3'X_1(X_1'X_1)^G & \underline{0} & I \end{bmatrix}$$

yields the reduced normal equations

$$(3.2) \quad \begin{bmatrix} X_1'X_1 & X_1'X_2 & X_1'X_3 \\ \underline{0} & X_2'D_1X_2 & X_2'D_1X_3 \\ \underline{0} & X_3'D_1X_2 & X_3'D_1X_3 \end{bmatrix} \begin{bmatrix} \underline{b}_1 \\ \underline{b}_2 \\ \underline{b}_3 \end{bmatrix} = \begin{bmatrix} X_1'\underline{y} \\ X_2'D_1\underline{y} \\ X_3'D_1\underline{y} \end{bmatrix}$$

where $D_1 = I - X_1(X_1'X_1)^GX_1'$ and $D_1X_1 = \underline{0}$.

From the results of Section 2 we have the sum of squares for regression given by

$$\begin{aligned} \text{SSR} &= \mathbf{y}' \mathbf{X}_1 (\mathbf{X}_1' \mathbf{X}_1)^{-1} \mathbf{X}_1' \mathbf{y} + \mathbf{y}' [\mathbf{D}_1 \mathbf{X}_2 | \mathbf{D}_1 \mathbf{X}_3] \begin{bmatrix} \mathbf{X}_2' \mathbf{D}_1 \mathbf{X}_2 & \mathbf{X}_2' \mathbf{D}_1 \mathbf{X}_3 \\ \mathbf{X}_3' \mathbf{D}_1 \mathbf{X}_2 & \mathbf{X}_3' \mathbf{D}_1 \mathbf{X}_3 \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{X}_2' \mathbf{D}_1 \mathbf{y} \\ \mathbf{X}_3' \mathbf{D}_1 \mathbf{y} \end{bmatrix} \mathbf{y} \\ &= \text{SS}_{\beta_1} + \text{SS}(\beta_2, \beta_3 / \beta_1) \end{aligned}$$

Again using the results of Section 2 with $\mathbf{X}_1 = \mathbf{D}_1 \mathbf{X}_2$ and $\mathbf{X}_2 = \mathbf{D}_1 \mathbf{X}_3$ we have

$$\text{SS}(\beta_2, \beta_3 / \beta_1) = \mathbf{y}' \mathbf{D}_1 \mathbf{X}_2 (\mathbf{X}_2' \mathbf{D}_1 \mathbf{X}_2)^{-1} \mathbf{X}_2' \mathbf{D}_1 \mathbf{y} + \mathbf{y}' \mathbf{D}_1 \mathbf{D}_{12} \mathbf{D}_1 \mathbf{X}_3 (\mathbf{X}_3' \mathbf{D}_1 \mathbf{D}_{12} \mathbf{D}_1 \mathbf{X}_3)^{-1} \mathbf{X}_3' \mathbf{D}_1 \mathbf{D}_{12} \mathbf{D}_1 \mathbf{y}$$

where $\mathbf{D}_{12} = \mathbf{I} - \mathbf{X}_2 (\mathbf{X}_2' \mathbf{D}_1 \mathbf{X}_2)^{-1} \mathbf{X}_2'$

so that

$$\text{SSR} = \text{SS}_{\beta_1} + \text{SS}(\beta_2 / \beta_1) + \text{SS}(\beta_3 / \beta_1, \beta_2)$$

where

$$\text{SS}_{\beta_1} = \mathbf{y}' \mathbf{X}_1 (\mathbf{X}_1' \mathbf{X}_1)^{-1} \mathbf{X}_1' \mathbf{y}$$

$$\text{SS}(\beta_2 / \beta_1) = \mathbf{y}' \mathbf{D}_1 \mathbf{X}_2 (\mathbf{X}_2' \mathbf{D}_1 \mathbf{X}_2)^{-1} \mathbf{X}_2' \mathbf{D}_1 \mathbf{y}$$

$$\text{SS}(\beta_3 / \beta_1, \beta_2) = \mathbf{y}' \mathbf{D}_1 \mathbf{D}_{12} \mathbf{D}_1 \mathbf{X}_3 (\mathbf{X}_3' \mathbf{D}_1 \mathbf{D}_{12} \mathbf{D}_1 \mathbf{X}_3)^{-1} \mathbf{X}_3' \mathbf{D}_1 \mathbf{D}_{12} \mathbf{D}_1 \mathbf{y}$$

Note that Lemma 1 shows that $\mathbf{D}_1 \mathbf{D}_{12} \mathbf{D}_1$ is unique and symmetric while idempotency follows from

$$\begin{aligned} (\mathbf{D}_1 \mathbf{D}_{12} \mathbf{D}_1)^2 &= [\mathbf{D}_1 - \mathbf{D}_1 \mathbf{X}_2 (\mathbf{X}_2' \mathbf{D}_1 \mathbf{X}_2)^{-1} \mathbf{X}_2' \mathbf{D}_1]^2 \\ &= \mathbf{D}_1 - \mathbf{D}_1 \mathbf{X}_2 (\mathbf{X}_2' \mathbf{D}_1 \mathbf{X}_2)^{-1} \mathbf{X}_2' \mathbf{D}_1 + \mathbf{D}_1 \mathbf{X}_2 (\mathbf{X}_2' \mathbf{D}_1 \mathbf{X}_2)^{-1} \mathbf{X}_2' \mathbf{D}_1 + \mathbf{D}_1 \mathbf{X}_2 (\mathbf{X}_2' \mathbf{D}_1 \mathbf{X}_2)^{-1} \mathbf{X}_2' \mathbf{D}_1 \\ &= \mathbf{D}_1 - \mathbf{D}_1 \mathbf{X}_2 (\mathbf{X}_2' \mathbf{D}_1 \mathbf{X}_2)^{-1} \mathbf{X}_2' \mathbf{D}_1 \\ &= \mathbf{D}_1 \mathbf{D}_{12} \mathbf{D}_1. \end{aligned}$$

Also note that from Lemma 1 we have $\mathbf{D}_1 \mathbf{D}_{12} \mathbf{D}_1 \mathbf{X}_2 = \mathbf{0}$.

The analysis of variance for the model (3.0) is thus

<u>Source</u>	<u>D.F.</u>	<u>Sum of Squares</u>
β_1 ignoring β_2, β_3	$\text{Rank}(X_1' X_1)$	$y' X_1 (X_1' X_1)^{-1} X_1' y$
β_2 adjusted for β_1 , ignoring β_3	$\text{Rank}(X_2' D_1 X_2)$	$y' D_1 X_2 (X_2' D_1 X_2)^{-1} X_2' D_1 y$
β_3 adjusted for β_1, β_2	$\text{Rank}(X_3' D_1 D_2 X_3)$	$y' D_1 D_2 X_3 (X_3' D_1 D_2 X_3)^{-1} X_3' D_1 D_2 y$
Error	$n - \text{Rank}(X' X)$	$y' [I - X_1 (X_1' X_1)^{-1} X_1' - D_1 X_2 (X_2' D_1 X_2)^{-1} X_2' D_1 - D_1 D_2 X_3 (X_3' D_1 D_2 X_3)^{-1} X_3' D_1 D_2] y$

Using the relations $D_1 X_1 = 0$, $D_1 D_2 X_2 = 0$ and the expressions (4) one can verify the expectations, variances and covariances of the sums of squares in the above analysis of variance which are given in Tables 3.1 and 3.2.

Table 3.1:

EXPECTATIONS OF SUMS OF SQUARES FOR MODEL (3.0)

Sum of Squares	σ^2	σ^2_3	σ^2_2	β Term
$SS(\beta_1)$	r_1	$Tr X_3' X_3 - Tr(X_3' D_1 X_3)$	$Tr(X_2' X_2) - Tr X_2' D_1 X_2$	$\beta_1' X_1' X_1 \beta_1$
$SS(\beta_2/\beta_1)$	r_2	$Tr(X_3' D_1 X_3) - Tr(X_3' D_1 D_{12} D_1 X_3)$	$Tr(X_2' D_1 X_2)$	---
$SS(\beta_3/\beta_2, \beta_1)$	r_3	$Tr(X_3' D_1 D_{12} D_1 X_3)$	---	---
SSE	$n - r_1 - r_2 - r_3$	---	---	---

where

$r_1 = \text{Rank } X_1' X_1$
 $r_2 = \text{Rank } X_2' D_1 X_2$
 $r_3 = \text{Rank } X_3' D_1 D_{12} D_1 X_3$

$D_1 = I - X_1 (X_1' X_1)^{-1} X_1'$
 $D_{12} = I - X_2 (X_2' D_1 X_2)^{-1} X_2'$

Table (3.2)

VARIANCES AND COVARIANCES FOR MODEL (3.0)

Sum of Squares	σ^4	σ^4_3	σ^4_2	$\sigma^2_2\sigma^2_3$	$\sigma^2_2\sigma^2_3$	$\sigma^2_2\sigma^2_2$	β_{Term}
$SS(\beta_1)$	$2r_1$	$2\text{Tr}[X_1'X_1(X_1'X_1)^G X_1'X_3]^2$	$2\text{Tr}[X_2'X_1(X_1'X_1)^G X_1'X_2]^2$	$4\text{Tr}[X_3'X_1(X_1'X_1)^G X_1'X_2]$ $X_2'X_1(X_1'X_1)^G X_1'X_3]$	$4\text{Tr}[X_3'X_1(X_1'X_1)^G X_1'X_3]$	$4\text{Tr}[X_2'X_1(X_1'X_1)^G X_1'X_2]$	$[4\beta_1'X_1'X_1\beta_1\sigma^2_1$ $+4\beta_1'X_1'X_2X_2'X_1\beta_1\sigma^2_2$ $+4\beta_1'X_1'X_3X_3'X_1\beta_1\sigma^2_3]$
$SS(\beta_2/\beta_1)$	$2r_2$	$2\text{Tr}[X_3'D_1X_2(X_2'D_1X_2)^G X_2'D_1X_3]^2$	$2\text{Tr}[X_2'D_1X_2]^2$	$4\text{Tr}[X_2'D_1X_3X_3'D_1X_2]$	$4\text{Tr}[X_3'D_1X_2(X_2'D_1X_2)^G X_2'D_1X_3]$	$4\text{Tr}[X_2'D_1X_2]$	
$SS(\beta_3/\beta_1, \beta_2)$	$2r_3$	$2\text{Tr}[X_3'D_1D_1D_1X_3]^2$			$4\text{Tr}[X_3'D_1D_1D_1X_3]$		
$SS(\beta_1)$			$2\text{Tr}[(X_2'D_1X_2)(X_2'X_2)]$	$4\text{Tr}[X_2'D_1X_3X_3'X_2]$			
$SS(\beta_2/\beta_1)$		$2\text{Tr}[(X_3'D_1X_2)(X_2'D_1X_2)^G(X_2'D_1X_3)X_3'X_1(X_1'X_1)^G X_1'X_3]$	$-2\text{Tr}[X_2'D_1X_2]^2$	$-4\text{Tr}[X_2'D_1X_3X_3'D_1X_2]$			
$SS(\beta_1)$		$2\text{Tr}[(X_3'D_1D_1D_1X_3)X_3'X_3]$					
$SS(\beta_3/\beta_2, \beta_1)$		$-2\text{Tr}[(X_3'D_1D_1D_1X_3)(X_3'D_1X_3)]$					
$SS(\beta_2/\beta_1)$		$2\text{Tr}[(X_3'D_1D_1D_1X_3)(X_3'D_1X_3)]$					
$SS(\beta_3/\beta_2, \beta_1)$		$-2\text{Tr}[(X_3'D_1D_1D_1X_3)]^2$					

All other covariances are zero.